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Semi-Annual Progress Report
for
A Study of Carbon Monoxide Distribution Determinations for a
Global Transport Model

by

Leonard K. Peters and James O. Manning
University of Kentucky
Lexington, Kentucky 40506

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A system of programs which model the chemistry and transport of carbon monoxide and methane in the earth's atmosphere on a global scale has been installed onto the NASA-Langley central scientific computer network. This system, the GLOBAL system, consists of a user-friendly set of procedural files which allow for simplified pre-processing, execution, and post-processing for all program elements. The package includes procedures for obtaining the NMC meteorological data, calculating the vertical winds to satisfy mass conservation, determining the boundary layer, and executing the transport/chemical model for carbon monoxide. In addition, plotting, saving to tape, and reading from tape routines have been developed.

Final modifications to the sub-programs for processing the input data for the transport/chemistry model have improved these data to more accurately reflect true atmospheric conditions. The growth and decay of the boundary layer corresponds to the solar zenith angle. Notwithstanding boundary conditions, mass conservation is within the requirements of the transport/chemistry model; i.e., the characteristic time for the divergence term is greater than the integration time step of the model.

The transfer of the transport/chemistry model from the NCAR DRAY

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system to the NASA-Landley VPS-32 system has now been completed; however, several formerly unrecognized complications have emerged. Initial modifications to input and manipulate actual meteorological data proved ineffective. These problems were traced to system idiosyncrasies and erroneous automatic vectorization. The source data for carbon monoxide and methane were originally stored on magnetic tape at NCAR (Boulder, CO). With multiple system changes, these data were lost and it became necessary to re-enter the data from original listings.

Several minor, but significant, errors in the computer algorithm were identified and corrected during the course of installing the transport/chemistry model onto the VPS-32 computer. The most perplexing of these errors was a incorrectly modified matrix solver. This subroutine correctly solved the matrix for a uniform wind field as had been used in previous operational runs; however, when the actual meteorological data were input, the subroutine could not correctly solve the matrix. Replacing this subroutine with a library routine proved to be an easy solution for this problem.

With these problems eliminated, progress toward complete installation led to two further difficulties: (1) the degree that mass conservation is maintained during temporal interpolations may not be within the limits of the model requirements; and (2) the boundary conditions at longitude 180° West appear not to correctly account for the correct mass flow.

The results of the model in regions far removed from the boundary condition are generally acceptable; however, sporadic errors do occur indicating the need for careful evaluation of the output. Various test

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cases have been completed where the chemistry and transport are separately and jointly suspended. These cases provide a basis for determining the cause of the errors. Further studies of the transport/chemistry model are to be accomplished at the University of Kentucky.

The attached flowcharts indicate the sequence of procedures which are executed for each twelve-hour period of meteorological data. The system is controlled by the main procedure named GLOBAL. The user is prompted for the program step which is to be executed. Automatic execution of the entire system could be attempted; however, a system malfunction could cause undetectable or costly errors. GLOBAL attaches and executes the appropriate procedure for the user-selected program.

The meteorological data must be processed by four FORTRAN programs: METRLGY for retrieving a subset ($5^{\circ} \times 5^{\circ}$ grid) of the packed meteorological data; WINDFLD for calculating the vertical wind field insuring mass conservation; BOUNDRY for determining the vertical eddy diffusivities and interpolating the meteorological data over a twelve-hour period; and TRANSPT for simulating the transport and chemistry model for carbon monoxide and methane. In addition, a fifth program, INITIAL, initializes the source and terrain data for the system.

As indicated in the flowcharts, each sub-system requires multiple job files to process the input and output files and queue the programs for execution on the appropriate computer. These job files have the following suffixes and function. The -PRC procedural file prompts the user for the date and hour for which the program will be executed and creates a -DAT file for input into the program. The -JOB job file routes the corresponding VPS-32 job file to that computer except for the

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METRLGY sub-system where the -JOB job file actually queues and controls this program. The -VPS job file queues and controls the execution of the four VPS-32 programs. And finally, the -SUB job file queues the output files for printing.

For each twelve-hour period, six output files are generated by the GLOBAL system: MDATA, which contains the NMC meteorological data from the METRLGY program; WDATA, which contains the results of the WINDFLD program; BDATA, which contains the results of the BOUNDRY program; KDATA, which contains the eddy diffusivities for the next time step of the BOUNDRY program; CDATA, which contains the carbon monoxide and methane for the next time step of the TRANSPT program; and TDATA, which contains the final results of the TRANSPT program.











